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Approximations of the Scattering Phase Functions of Particles

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ABSTRACT

Based on anomalous diffraction theory and the modified Rayleigh-Debye approximation, a physically realistic model in bridging form is described to approximate the scattering phase function of particles. When compared with the exact method, the bridging technique reported here provides a reasonable approximation to the Mie results over a broader range of angles and size parameters, and it demonstrates the advantage of being computationally economic. In addition, the new phase function model can be essentially extended to other shapes and conveniently used in more complicated scattering and emission problems related to the solutions of the radiative transfer equations.

Key words: small light scattering, particles, phase function, bridging technique

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1. Introduction

The scattering phase function is one of the basic inputs in various radiative transfer models that describes the normalized angular distribution of scattered radiative energy and also represents the probability for radiation propagating from a given direction to be scattered into an elementary solid angle about another direction. In principle, the phase function is determined by solutions of the Maxwell equations for the interaction between the radiation field and particulate medium, and its quantitative calculation can be performed accurately by means of miscellaneous analytical and numerical techniques aimed at the electromagnetic scattering problems. These methods, including the separation of variables method, integral equation method, T-matrix method, point matching method, superposition method, finite element method and finite difference time domain method, have been recently reviewed by Wriedt (1998), Mishchenko et al.(2000), Liou (2002), and Kahnert (2003). However, the comprehensive investigation of solutions to electromagnetic scattering problems has been confined to a few simple shapes. Generally for the complex shaped particles, the common trick is employing the equivalent sphere model so as to make the Lorenz-Mie theory available. As has been pointed out, even with this simplifying assumption, strong angular oscillations and considerable computation time in the calculation may occur (Modest, 2003), which will enormously complicate the analysis of the radiative transfer at a given wavelength. This inconvenience has led to the design of a simple but accurate approximate phase function.

So far, quite a few models have been developed to approximate the scattering phase function. Henyey and Greenstein (1941) proposed an empirical model (the so-called HG phase function) to describe the scattering of radiation in a galaxy. This expression, with g (the asymmetric factor) as a single free parameter, has been widely used in atmospheric sciences because of its simple and analytic form. However, it can become highly inaccurate for some values of the particle size parameter and refractive index. To improve the precision of the HG phase function, some modifications and extensions have been suggested, which include the modified HG phase function (Cornette and Shanks, 1992; Draine, 2003), the two-parameter phase function (Reynolds and McCormick, 1980), and the three-parameter phase function (Irvine, 1965; Kattawar, 1975). Besides the HG-type approximations, there are other valuable forms which have been proposed, e.g., by Chu and Churchill (1955), McKel-

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lar and Box (1981), Fournier and Forand (1994), Liu (1994), Sharma and Roy (2000), Sharma et al.(1998), and Caldas and Semião (2001). However, the abovementioned phase functions cannot describe the asymptotic limit for small and large particles simultaneously.

In this paper, we present a new scattering phase function valid for various sizes by the bridging technique. In section 2, the asymptotic behavior of the phase function formula is discussed and a new bridging function for it is developed. Section 3 contains comparisons of the new approximation to the exact method for spheres. The main results are summarized in section 4.

2. Development of the phase function formulas

Consider the general scattering problem of an arbitrarily shaped particle characterized by volume V and projected area P. As is well known, the scattering properties of particles that are optically small enough can be represented by the Rayleigh-Debye approximation (RDA), and those that are optically large enough can be approximated by anomalous diffraction theory (ADT). The primary object of this article is to combine the two asymptotic approximations into a general expression that is capable of describing the phase function for particles of all sizes.

2.1 *Small particle limit*

The RDA, otherwise known as the Rayleigh-Gans approximation or Born approximation (Irvine, 1965), as a powerful tool, is widely applied to the problems of light scattering by small particles. General conditions of the validity of the RDA are $kd|m-1| \ll 1$ and $kd|m-1| \ll 1$, where d represents the characteristic particle size, m is the complex index of refraction of particle relative to the medium，and k is the wave number. These conditions imply that the particles are assumed to be not too large compared to the wavelength of radiation (although they may be larger than in the case of Rayleigh scattering) and optically "soft". The fundamental assumption of the RDA is that each volume element of the scattering object is excited only by the incident field, and the electric field inside the scatterers is equal to the incident field. This simplified assumption leads to significant analytical progress in many specific cases. On the other hand, some improvements and extensions for RDA have been made already (Acquista, 1976; Khlebtsov, 1984; Khlebtsov and Melnikov, 1991; Khlebtsov et al., 1991; Muinonen, 1996). If the particle irradiated by unpolarized light is assumed homogeneous and isotropic, the scattering phase function in the small particle limit, $p(\theta)_{\text{small}}$ can be expressed as

$$p(\theta)_{\text{small}} = a|b_1|^2(1+\cos^2\theta)\ , \qquad (1)$$

where θ is the scattering angle, a is the normalization constant, and b_1 is the form factor, which is given by

$$b_1 = \frac{1}{V}\int \exp[i(\boldsymbol{k}_{\text{i}} - \boldsymbol{k}_{\text{s}})\cdot \boldsymbol{r}']d^3\boldsymbol{r}'\ , \qquad (2)$$

where $i=\sqrt{-1}$ is the imaginary unit, $\boldsymbol{k}_{\text{i}}$ and $\boldsymbol{k}_{\text{s}}$ are wave-vectors of the incident field and scattering field, respectively, $d^3\boldsymbol{r}'$ is the volume element at the point $\boldsymbol{r}'(x',y',z')$ within scatterer. However, Shimizu (1983) pointed out that Eq. (2) does not yield the correct angular position for the extrema in the scattering curves. Saxon (1955) and Gordon (1985) discussed and suggested respectively a modified RDA (MRDA) method, which allows the refractive index of the particle to enter the calculation, whereas in the unmodified RDA the scattering results are independent of m. Unfortunately, the MRDA scheme is not exact enough for particles comparable in size to wavelength, so here we design a new scheme to improve the original MRDA and rewrite Eq. (1) as

$$p(\theta)_{\text{small}} = a_0[t|b_1|^2 + (1-t)(|b_2|+\gamma)^2](1+\cos^2\theta) \qquad (3)$$

with

$$\begin{cases} b_2 = \dfrac{1}{V}\displaystyle\int \exp[i(m\boldsymbol{k}_{\text{i}} - \boldsymbol{k}_{\text{s}})\cdot \boldsymbol{r}']d^3\boldsymbol{r}' \\ t = \exp[-c_1 x_{\text{vp}}^3] \\ \gamma = \dfrac{x_{\text{vp}}^{9/2}}{(200+x_{\text{vp}}^6)(1+m^2-2m\cos\theta)^{3/4}}\ . \end{cases} \qquad (4)$$

In Eq. (4), $c_1 = 5Re[(m-1)/8]$, Re represents the real part of a complex quantity $x_{\text{vp}} = 3kV/(4P)$ is the equivalent-sphere size parameter. Then new normalized factor a_0 is determined according to relation:

$$\int p_{\text{small}}(\theta)d\Omega = 1\ , \qquad (5)$$

where $d\Omega = \sin\theta d\theta d\varphi$ is the element of solid angle and the integration is over all scattering angles.

2.2 *Large particle limit*

The traditional ADT is a widely used Eikonal-type approximation (Van de Hulst, 1957; Chen, 1984) and was initially developed to calculate the extinction and absorption cross section for large optically soft spheres. Xu and Alfano (2003) put a statistical interpretation on it recently. ADT presumes that the index of refraction is close to unity and that the size parameter is large enough. This assumption implies that the refraction and the reflection are negligible as the ray passes through the particles, and it allows simple analytical expressions for many geometrical shapes. These consist of spheres (Van de Hulst, 1967), spheroids (Greeberg and Meltzer, 1960; Fournier and Evans, 1991), ellipsoids (Streekstra et al., 1994), cubes (Napper, 1967; Maslowska et al., 1994), prismatic columns

(Chylek and Klett, 1991a, 1991b), hexagonal crystals (Sun and Fu, 2001), infinite cylinders (Gross and Latimer, 1970), elliptical cylinders (Fournier and Evans, 1996), finite circular cylinders (Liu et al., 1998), fractal clusters (Meeten, 1982), and arbitrary shapes (Zhao and Hu, 2003). Like other high-energy approximations (Perrin and Chiappetta, 1985, 1986; Bourrly et al., 1989; Klett and Sutherland, 1992), ADT also possesses the ability to describe the angular distribution of scattering energy. Briefly, the scattering phase function in the larger particle limit, $p(\theta)_{\rm large}$ has the form:

$$p(\theta)_{\rm large} = \frac{|f(\boldsymbol{k}_{\rm i},\ \boldsymbol{k}_{\rm s})|^2}{C_{\rm sca,ad}}\ , \tag{6}$$

where $C_{\rm sca,ad} = \int |f(\boldsymbol{k}_{\rm i},\ \boldsymbol{k}_{\rm s})|^2 d\Omega$ is the scattering section, and the unpolarized scattering amplitude function $f(\boldsymbol{k}_{\rm i},\ \boldsymbol{k}_{\rm s})$ is expressed by Zhao (2003):

$$f(\boldsymbol{k}_{\rm i},\ \boldsymbol{k}_{\rm s}) = -\frac{ik}{2\pi}\int\{\exp[i(\boldsymbol{k}_{\rm i}-\boldsymbol{k}_{\rm s})\cdot\boldsymbol{r}']\times \frac{\partial}{\partial z'}\left\{\exp\left[ik\int_{-\infty}^{z'} dz''(m-1)\right]\right\} d^3\boldsymbol{r}'\ . \tag{7}$$

In above equation, $z'' = \boldsymbol{r}''\cdot\hat{\boldsymbol{e}}_{z'}, \boldsymbol{r}'' = \boldsymbol{r}-\boldsymbol{r}'$ and $\boldsymbol{r}''//\boldsymbol{r}$, $\boldsymbol{r}$ is position vector at the observation point far from the particle, $\hat{\boldsymbol{e}}_{z'}$ is the unit vector along z' axis, and the integration is done over all space. Additionally, it should be noted that the scattering section can also be approximated by

$$C_{\rm sca,ad} = \iint |1-\exp[ik(m-1)l]|^2 dP\ , \tag{8}$$

where l represents a geometrical path of a given ray path through the particle, dP is the area element of the projection on the plane perpendicular to the direction of the light ray, and the integration domain is over the whole projected area P.

2.3 *Bridging function*

As the particle size approaches zero and infinity, the corresponding phase function expressions approach the MRDA and the ADT expressions, respectively. A bridging function is required for the intermediate particles. The bridging function should satisfy the following two conditions: (1) it should be able to provide reasonably good approximation over the range between the so-called Mie scattering region and the geometrical optics region; (2) it can be applied to a variety of particle shapes, sizes and all scattering angles. In this paper, the following simple bridging function is selected:

$$f(\xi) = f_1(\xi)F_1 + f_2(\xi)F_2\ , \tag{9}$$

where $f_i (i = 1, 2)$ denotes a function. This function can be used to smoothly bridge the transition between two given functions F_1 and F_2 when the independent variable ξ is increasing if

(a) $f_1(\xi) \to 1$, for small ξ
(b) $f_1(\xi) \to 0$, for large ξ
(c) $f_1(\xi) + f_2(\xi) = 1$

Clearly, convenient choices for our purpose are

$$F_1 = p(\theta)_{\rm small}\ , \tag{10}$$

$$F_2 = p(\theta)_{\rm large}\ , \tag{11}$$

For simplicity, it is considered that independent variable ξ can be approximated by equivalent-sphere size parameter $x_{\rm vp}$, and function $f_1(x_{\rm vp})$ represents exponential decay:

$$f_1(x_{\rm vp}) = \exp(-c_2 x_{\rm vp}^3)\ . \tag{12}$$

By extensive trial and error for spherical particles, we find that the optimal values of c_2 over all size parameters can be given by $c_2 = 0.0128\ {\rm Im(m)}$. In the previous section, a similar bridging technique has been employed to obtain Eq. (4). Finally, the complete formulation for the phase function, which has two asymptotes as its limits, can be expressed by

$$p(\theta) = \exp(-c_2 x_{\rm vp}^3)p(\theta)_{\rm small} + [1-\exp(-c_2 x_{\rm vp}^3)]p(\theta)_{\rm large}\ . \tag{13}$$

3. Comparisons with exact results

To evaluate the accuracy of the proposed phase function, we compare it with the exact Lorenz-Mie phase function and HG approximate phase function. The simplification here used for spheres is listed below:

(I) Form factors in MRDA

$$b_1 = b(\xi_1),\ \ b_2 = b(\xi_2) \tag{14}$$

where $\xi_1 = 2x\sin(\theta/2)$, $\xi_2 = x(1+m^2-2m\cos\theta)^{1/2}$, $x = ka, a$ is the radius of the particle, and function $b(\xi)$ is defined as

$$b(\xi) = \frac{3(\sin\xi - \xi\cos\xi)}{\xi^3}\ . \tag{15}$$

(II) Scattering amplitude function in ADT

$$f(\theta) = \frac{-ix(m-1)}{m-1+2\sin^2(\theta/2)}\times \int_0^{\pi/2} d\tau[\sin\tau\cos\tau J_0(x\cos\tau\sin\theta)\times \{\exp[-i2x\sin^2(\theta/2)\sin\tau] - \exp[i2x\sin\tau((m-1)+3\sin^2(\theta/2))]\}]\ , \tag{16}$$

where τ is parameter angle, and J_0 is the zeroth order Bessel function.

(III) The scattering section in ADT

$$C_{\rm sca,ad} = 2P\{Re[Q[i(m-1)]] - Q[-2Im(m-1)]\}\ , \tag{17}$$

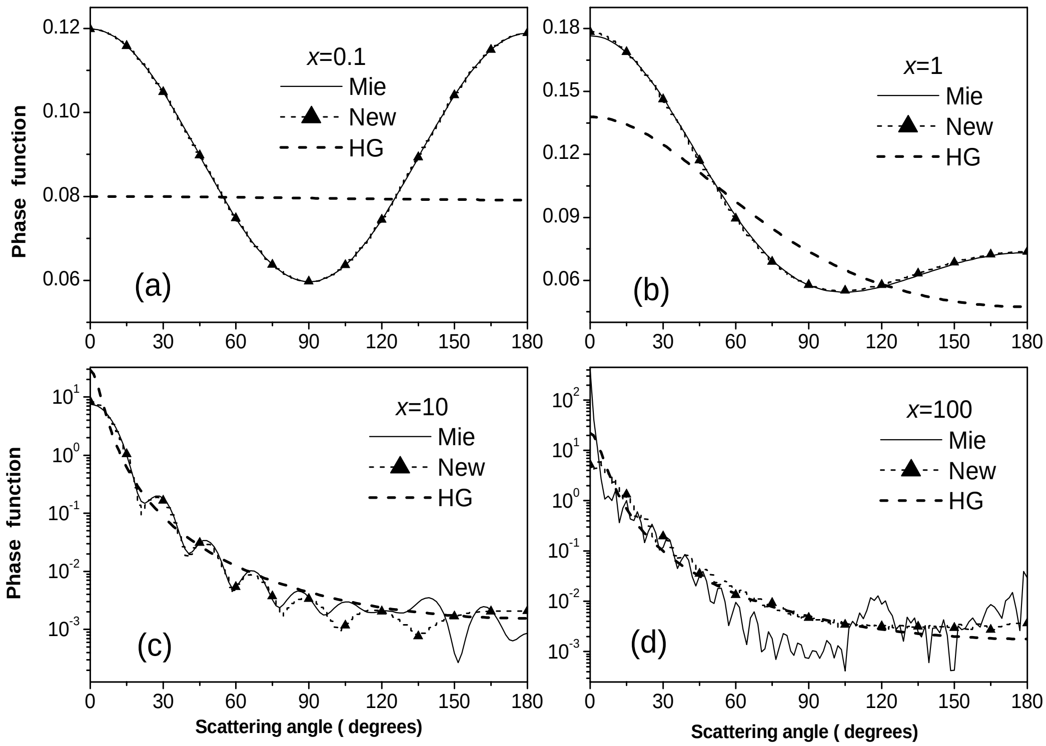

Fig. 1. Comparisons of the new phase function with the Mie phase function and the HG phase function for x=0.1, 1, 10，and 100 and relative refractive index $m = 1.2 + 0.0i$.

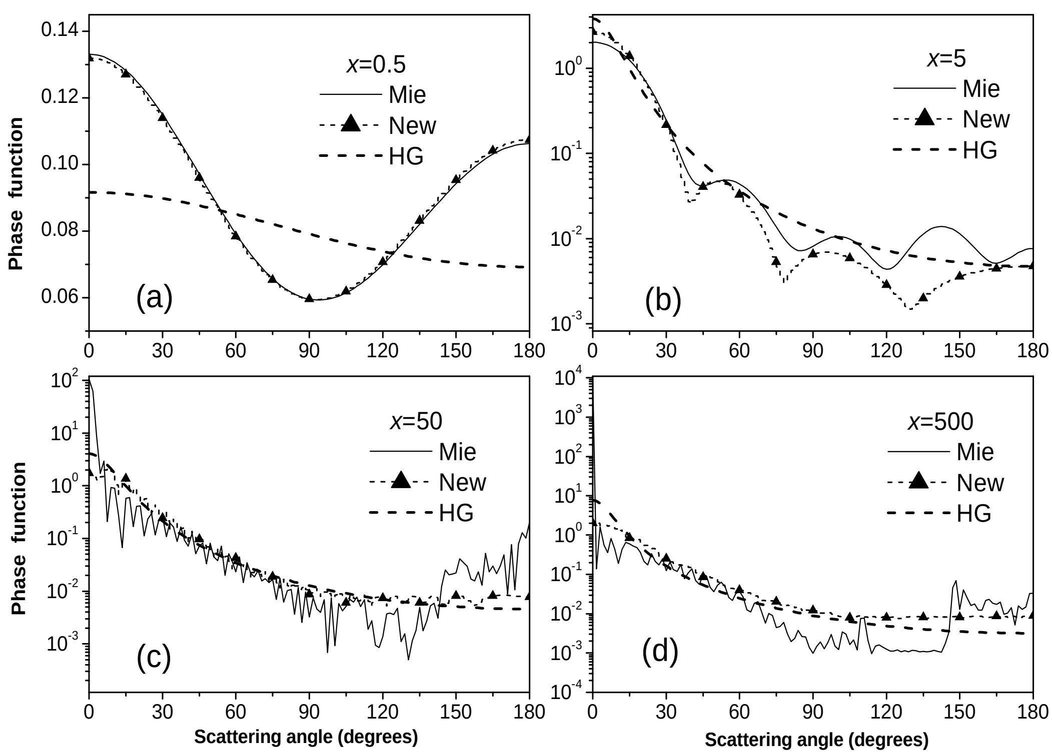

Fig. 2. Same as Fig. 1 but for x=0.5, 5, 50, and 500 and $m = 1.2 + 0.0i$.

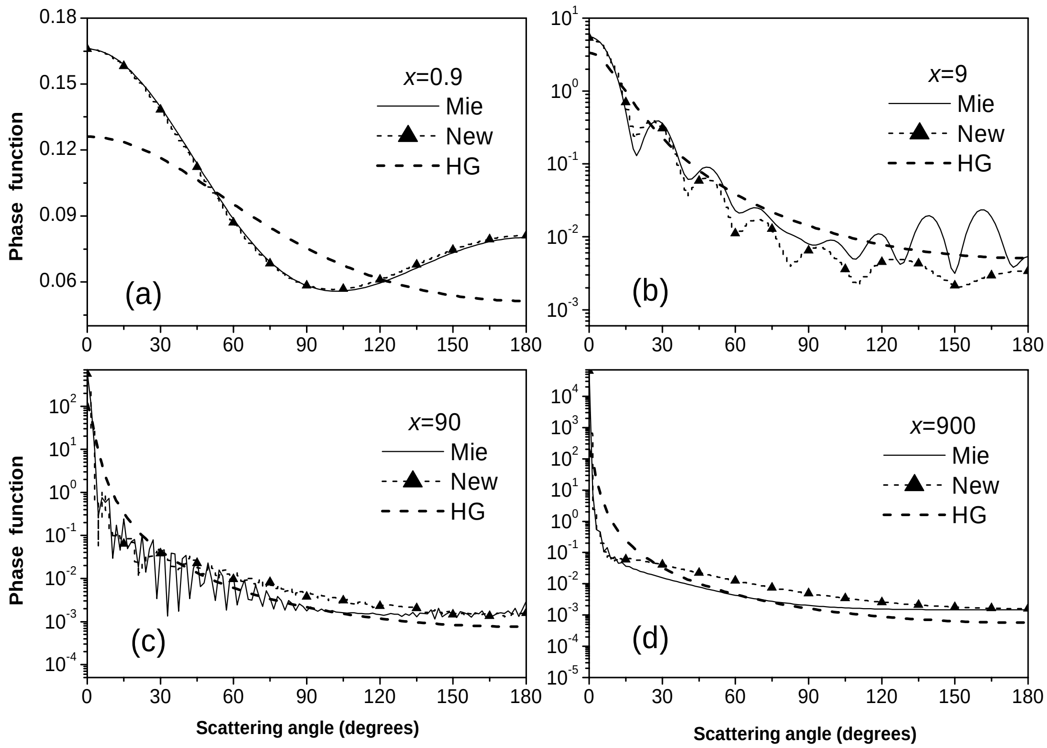

Fig. 3. Same as Fig. 1 but for x=0.9, 9, 90, and 900 and $m = 1.33 + 0.0i$.

where Im represents the imaginary part of a complex quantity, and function $Q(\xi)$ is defined by

$$Q(\xi) = 2\left[\frac{1}{2} - \frac{\exp(\xi x)}{(\xi x)} - \frac{1-\exp(\xi x)}{(\xi x)^2}\right] . \qquad (18)$$

Figure 1 demonstrates the comparison for different size parameters x=0.1, 1, 10, 100 and the complex relative index of refraction $m = 1.2 + 0.0i$. Figure 2 shows the results of the agreements for x=0.5, 5, 50, 500 and $m = 1.2 + 0.0i$. The case of absorption for size parameters x=0.9, 9, 90, 900 and $m = 1.33 + 0.01i$ is displayed in Fig. 3. It is clear from the comparisons in these figures that new phase function model is a very good representation of the exact phase function at small and moderate sizes. In contrast, HG shows poor agreement. As the size parameter and the real part of the refractive index of the particle increase, many lobe patterns begin to appear in the curve of the real phase function; accordingly, it will be more difficult to reproduce them well and accurately. As it stands, the new model of the phase function is able to provide correctly the descriptions of the forward peak and backscattering behavior for the larger imaginary refractive indexes and larger sizes. Liu et al.(1998) discussed similar results for cylinders in ADT.

4. Conclusions

A physically realistic model based on a bridging technique is proposed to calculate the phase function for unpolarized light by particles over a wide range of sizes. Comparisons of the new expressions with the results from the exact theory and other approximations (HG phase function) are made for spherical particles. It is obvious that the new model achieves good agreements at all scattering angles and constitutes a substantial improvement over the HG approximate phase functions. Also, it leads to analytic expressions for small and even moderate sized α parameters, and it provides a simple way of predicting the variation of relative intensity with scattering angle for radiation incident upon aerosol particles suspended in the atmosphere. The new method will be sufficiently accurate for polydisperse particles and can be potentially applied to particles of other shapes and sizes. So, it is worthwhile to investigate further the practical performance of this new phase function in the multiple scattering problems under various physical conditions.

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